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PARTIAL DISCRETIZATION AND PRESERVATION RELATIONS

DIEGO B. HERNÁNDEZ

Departamento de Ingeniería
Universidad Autónoma Metropolitana
Iztapalapa, Apdo. 55-534
09340 México DF
México

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Abstract—Partial discretization as a means for simplifying mathematical models is examined in detail. The main aim of this endeavor is to reconcile the approximate character of this model simplification technique with some fairly recent system theoretic developments, in which valid simplification is characterized in terms of certain preservation relations. To this end, a model is constructed for systems of interest in blood physiology and chemical engineering, then this model is subjected to all sorts of manipulations, including partial discretization. Out of this analysis, there emerges the notion of approximate preservation relation, which characterizes validity of this approximate simplification procedure.

1. INTRODUCTION

It has been pointed out recently [1] that physical phenomena consist of changes in the spatial–temporal distribution of certain attributes of interest (e.g., temperature, concentration, pressure, etc.) subject to certain modes of interaction with the external world. Their mathematical descriptions must include representatives of all these elements, hence a mathematical model must be a collection of objects (nonempty sets) of the form

$$\langle T, S, A, E, \Omega \rangle, \tag{1.1}$$

subject to the following interpretation: here the elements of T represent *time*, those of S are representatives of points in *space* and A consists of possible values for the *attributes*. Normally $T \subset \mathbf{R}$, $S \subset \mathbf{R}^d$ and $A \subset \mathbf{R}^n$ for some $d \leq 3$, $n \in N$. As to E, its elements are the possible instantaneous spatial distributions of attributes, hence it consists of A valued functions on S, the attribute *profiles*. Finally each $\omega \in \Omega$ is a function from T into E, its value $\omega(t)$ being "the profile at time t." Now not all such functions $\omega: T \to E$ are included in Ω, same as not all $e: S \to A$ are acceptable and therefore belong to E. Which temporal *evolutions* ω constitute Ω and which profiles constitute E is at the heart of the modelling process, the choice being ultimately dictated by the modeller's knowledge of the physical system of interest. See Sec. 2 below for an example in which a model such as (1.1) is constructed for each of two different physical situations. Those situations involve transport phenomena and chemical reaction in a cylindrical vessel, one of them a biological system. See [1] for a discussion on the relation of

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(1.1) to physical reality in a general context, including the role played by determinism and causality.

On the other hand, many mathematical models like (1.1)—the example in Sec. 2 among them—can be taken into the form of a *dynamical system* [2]

$$\langle T, U, X, Y, \mathcal{U}, \delta, \lambda \rangle \tag{1.2}$$

where T, U, X, Y, and $\mathcal{U}$ are nonempty sets (T as before), δ and λ are functions. The elements of U, X, and Y are called *input* values, internal *states*, and *output* values, respectively, and $\mathcal{U}$ is a collection of U valued functions defined on T (the input trajectories). If $x \in X$ and u_{ab} is the restriction of $u \in U$ to interval $[a, b)$, then $\delta(x, u_{ab})$ is the state arrived at when the initial (at $t = a$) state is x and input u is applied over (a, b). Finally, $\lambda(x) \in Y$ is the output detected when the internal state is x. A collection like (1.2) is a *dynamical system* [2] if

$$\delta(x, u_{sl}) = \delta(\delta(x, u_{sr}), u_{rt}), \quad s < r < t,$$

a condition that must be introduced in order to avoid inconsistencies. See Sec. 3 below where the model (1.1) previously constructed in Sec. 2 is cast into the shape of a dynamical system like (1.2). That system is seen to be specified in terms of linear ordinary differential equations with trajectories in X (which is infinite dimensional in this case) similar to

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx, \end{aligned} \tag{1.3}$$

A, B, and C being appropriate linear operators. Zeigler [3, Chap. 10] develops a theory of valid simplification for systems such as (1.2) to be replaced by a "simpler" system

$$\langle \bar{T}, \bar{V}, \bar{X}, \bar{Y}, \bar{U}, \bar{\delta}, \bar{\lambda} \rangle. \tag{1.4}$$

Assuming, for the sake of simplicity, that $\bar{T} = T$, $\bar{U} = U$, $\bar{Y} = Y$, $\bar{\mathcal{U}} = \mathcal{U}$, the simplification is done by means of mappings $P : X \to \bar{X}$ and $Q : Y \to Y$, both of them onto. If (1.2) is specified in terms of linear differential equations such as (1.3)—and that is the case for our example—then it is convenient to restrict ourselves to linear P and Q, since then (1.4) will also be specified in terms of differential equations, namely,

$$\begin{aligned} \dot{\bar{x}} &= \bar{A}\bar{x} + \bar{B}u \\ \bar{y} &= \bar{C}\bar{x}. \end{aligned}$$

In this particular context, simplification P, Q is valid [3, p. 269] if and only if the following preservation relations hold:

$$\begin{aligned} PA &= \bar{A}P \\ PB &= \bar{B} \\ QC &= \bar{C}P. \end{aligned}$$

Many examples are given in Sec. 3 illustrating this type of valid simplification on our model example constructed in Sec. 2. Finally, Sec. 4 is devoted to a very important type of model simplification, namely, *discretization*, which is not valid in the sense just mentioned, but nevertheless merits all possible attention in view of its practical importance [4, Chap. 10]. To

simplify matters, assume $B = 0$, $C = 0$ in (1.3), so that discretization amounts to the replacement

$$X \to X_h \quad \text{and} \quad \dot{x} = Ax \to \dot{x}_h = A_h x_h.$$

Here h is the "discretization parameters" (e.g., the mesh size) and X_h is finite dimensional even if X is infinite dimensional. Validity would require the preservation relation

$$P_h A = A_h P_h, \tag{1.5}$$

where $P_h: X \to X_h$ accomplishes the discretization. For example, if x is a continuous real function on $[0, 1]$ and $h = 1/N$, then $X_h = \mathbf{R}^{N+1}$ and

$$P_h x = (x(ih), \quad i = 0, 1 \ldots N). \tag{1.6}$$

Several examples are given in which (1.5) does not hold. Instead one gets at most the approximate preservation relation

$$\lim_{h \to 0} \|P_h A x - A_h P_h x\|_h = 0, \quad x \in X, \tag{1.7}$$

where $\| \ \|_h$ is a norm on X_h. It is possible to show that (1.6) satisfies

$$\|P_h x\|_h \uparrow \|x\| \text{ as } h \to 0, \quad x \in X, \tag{1.8}$$

where

$$\|x\| = \max_{0 \le z \le 1} |x(z)|,$$

see [5, p. 225] for the details. Then, by a well known theorem due to Trotter [6; 5, Chap. 6], (1.7) and (1.8) suffice to guarantee that

$$x_h(t) \to x(t) \text{ as } h \to 0 \tag{1.9}$$

provided $x_h(0) = P_h x(0)$. Moreover, convergence in (1.9) is uniform in bounded t-intervals. Note that $x_h(t) \in X_h$, $x(t) \in X$, and $X_h \neq X$, hence (1.9) actually means

$$\lim_{h \to 0} \|x_h(t) - P_h x(t)\|_h = 0. \tag{1.10}$$

This result of Trotter has been the subject of much subsequent work. See [7, Theorem 4.6] for the so-called Trotter–Kato theorem, as well as [8, 9, 10] for its use in developing approximation theories of interest in control and identification. Kurtz has extended Trotter's result [11, 12] and applied it to stochastic approximation extensively during the last decade [13]. In view of the availability of these results, it is most important to prove approximate preservation relations such as (1.7) when simplifying mathematical models.

2. TRANSPORT AND REACTION IN A CYLINDER

The ideas referred to in the introduction are rather general and some insight might result from applying them to a particular example. However, it must be borne in mind that the ideas

themselves will not be less general in the treatment following this section, only they will be embodied in the concrete situation to be described below. This situation is interesting for its own sake and some of its variants (e.g., the Graetz problem) have a rather venerable history. For an enlightening discussion on these topics the reader is referred to the well documented account in [14]. Consider the following descriptions:

(a) *A tube wall reactor* [15]

A chemical reaction intended to produce a desired product A_2 from a single reactant A_1 takes place in the presence of a catalyst according to the reaction

$$A_1 \xrightarrow{k} A_2.$$

(A much more interesting reaction scheme is dealt with in [15], but this one will suffice for our purposes.) The reaction releases a considerable amount of heat. Hence, from the point of view of heat removal, a tubular reactor with the catalyst placed on the tube wall seems a convenient arrangement [15]. Determine the spatial distribution of each substance, assuming steady isothermal operation.

(b) *Hemostasis and thrombosis*

Platelets carried in bloodstream adhere to sites of intravascular injury and to artificial organs, then they release agents like ADP into the bloodstream [16]. Both platelets and releasable agent accumulate on the inner surface of the blood vessel. Measurements have been made of the concentration profiles of both platelets and releasable agents along the vessel, as well as of the flux of released material into the bloodstream [17]. Determine the spatial distribution of released agent under steady conditions.

Different as these situations may seem, they are amenable to a unified mathematical treatment. Let's concentrate on this common mathematical structure which will be presented as an illustration of the general concepts given in the first few sections of [1]. For, let's begin by introducing some simplifying assumptions, listed below:

A1. The cylinder (tube or blood vessel) is very long.
A2. Operation is steady and there are no temperature variations.
A3. Fluid conditions at the tube entrance are known and the fluid is uniform prior to entrance.
A4. The tube wall reactor is packed with inert pellets in order to enhance mass transfer to and from the wall surface. Therefore plug flow can be assumed in the axial direction [15].
A5. In the blood vessels flow is laminar, with fully developed parabolic velocity profile in the region of interest [17].
A6. There is cylindrical symmetry, i.e., physical properties do not depend on orientation within the cylinder.
A7. Mass transport obeys Fick's law, with constant diffusion coefficients.
A8. Mass dispersion in the axial direction can be neglected in comparison with convection transport.

See [15] for a more complete statement of the assumptions underlying the modelling of the tube wall reactor, also [16] and [17] on platelet adhesion and release. These seven assumptions will form the basis of our treatment here.

Assumption A2 translates immediately in that a suitable choice for "time set" [1] is

$$T := \{0\}, \tag{2.1}$$

which we can ignore in the sequel. Moreover only mass balances will be required. In turn,

assumptions A1 and A6 translate into a space set [1] given by

$$S := [0, \infty) \times [0, a], \tag{2.2}$$

where a is the cylinder radius measured in suitable units. Points in S will be denoted by (z, r), coordinates denoting position along the cylinder axis and radial distance from it, respectively. Note that the cylinder is assumed to be infinitely long, in response to A1.

In both cases the attribute of interest is concentration of two species: chemical A_1 and A_2 in (a), platelets and released agent in (b), also identified with A_1 and A_2, respectively. Therefore it seems appropriate to take

$$A := \mathbf{R}^2 \tag{2.3}$$

for attribute set [1]. Elements of A will be denoted by (C_1, C_2), C_1 being the concentration of reactant (platelets), C_2 that of the desired product (released agent).

It is convenient to restrict our attention to profiles $e : S \to A$ which are twice continuously differentiable in order to set up the appropriate conservation equations. The value of one such profile at a given point $(z, r) \in S$ will be denoted by $(C_1(z, r), C_2(z, r))$, and A3 can be translated into the statement that

$$C_i(0, r) = C_i^0, \quad 0 \le r \le a, \quad i = 1, 2 \tag{2.4}$$

where C_1^0 and C_2^0 are the reactant (resp. platelet) and desired product (resp. released agent) concentrations at the tube inlet. To prevent explosive behaviour, it is convenient to supplement (2.4) by

$$\lim_{z \to \infty} C_i(z, r) \text{ exists}, \quad 0 \le r \le a, \quad i = 1, 2. \tag{2.5}$$

By A4 and A5, the local fluid velocity is independent of the axial coordinate and it is given by

$$v(r) = 2\bar{v}\left[1 - \left(\frac{r}{a}\right)^2\right] \tag{2.6}'$$

in the case of blood flow, by

$$v(r) = \bar{v} \tag{2.6}''$$

for the tube wall reactor, $\bar{v}$ being the average velocity computed in terms of volumetric flow and cross section.

Standard conservation-law type of arguments [18] lead us to translate A2 and A7 into the statements that

$$v(r)\frac{\partial C_i}{\partial z} = \bar{D}_i \frac{\partial^2 C_i}{\partial z^2} + \frac{D_i}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right), \quad i = 1, 2, \tag{2.7}$$

plus

$$-D_i \frac{\partial C_i}{\partial r}(z, 1) = h_i[C_i(z, 1) - C_{i,w}(z)], \quad i = 1, 2, \tag{2.8}$$

where D_i and $\bar{D}_i$ are the diffusion coefficients in the radial and axial directions, respectively, and h_i is a mass transfer coefficient at the wall, for component i. In (2.8), $C_{i,w}$ denotes the concentration profile at the wall, also of component i. Let

$$f(C_{1,w}) := \text{rate of production of } A_2 \text{ when surface concentration of } A_1 \text{ is } C_{1,w}$$

$$J(z) := \text{rate of deposition of } A_2 \text{ on wall,}$$

both rates measured in mass per unit area per unit time units. Then, the observations that whatever A_1 that diffuses to the wall reacts and whatever A_2 that does not stay at the wall diffuses into the mainstream can be translated as

$$f(C_{1,w}(z)) = h_1[C_1(z, a) - C_{1,w}(z)], \qquad z \geq 0 \tag{2.9}$$

$$f(C_{1,w}(z)) = h_2[C_{2,w}(z) - C_2(z, a)] + J(z), \quad z \geq 0. \tag{2.10}$$

Note that these last two equations can be solved for the concentrations at the wall, giving each $C_{i,w}(z)$ in terms of $C_1(z, a)$ and $C_2(z, a)$. These can in turn be plugged into (2.8), thus giving rise to the nonlinear boundary conditions

$$D_1 \frac{\partial C_1}{\partial r} + h_1[C_1 - \psi(C_1)] = 0, \quad z \geq 0, r = a, \tag{2.11}$$

$$D_2 \frac{\partial C_2}{\partial r} + f(\psi(C_1)) = J(z), z \geq 0, r = a, \tag{2.12}$$

where ψ satisfies

$$f(\psi(x)) = h_1[x - \psi(x)]. \tag{2.13}$$

Finally, dictated by the fact that the differential operator on the right hand side of (2.8) is not regular at $r = 0$ the following technical condition must be introduced:

$$C_i(z, 0) \text{ is finite, } z \geq 0, \quad i = 1, 2. \tag{2.14}$$

These conditions fully specify the set of all admissible profiles, namely,

$$E := \{e \in C^2(S, A) : (2.4\text{–}5), (2.7), (2.11\text{–}12), (2.14)\}. \tag{2.15}$$

Due to (2.1) only time invariant evolutions must be considered, hence we can identify each of them with the corresponding profile and take

$$\Omega := E. \tag{2.16}$$

The defining relations (2.1–3) and (2.15–16) specify all the elements in the mathematical model

$$\langle T, S, A, E, \Omega \rangle \tag{2.17}$$

arrived at under assumptions A1–A7 and common to both situations described at the beginning of this section, taking (2.6) into account.

Assuming all parameters in the model (a, C_1^0, C_2^0, D_1, $\bar{D}_1$, D_2, $\bar{D}_2$, h_1, h_2, $\bar{v}$, and k) are known,

the question of characterizing steady state behaviour can be expressed as follows:

$$\text{"Given } J\text{, find } e \in E\text{."} \tag{2.18}$$

This task can be accomplished by the following series of steps:

1. Solve (2.13) to obtain ψ.
2. Solve the partial differential equation (2.7) with the boundary conditions (2.4–5), (2.14) for $i = 1$ and (2.11), thus obtaining C_1.
3. Solve equation (2.7) with boundary conditions (2.4–5), (2.14) for $i = 2$ together with (2.12), with C_1 as obtained in step 2.

The execution of these steps becomes considerably simpler if linear kinetics is assumed,

$$f(C_{1,w}) = kC_{1,w}. \tag{2.19}$$

Then, step 1 yields

$$\psi(x) = \frac{h_1}{k + h_1} x$$

so that (2.11) reduces to

$$D_1 \frac{\partial C_1}{\partial r} + \frac{kh_1}{k + h_1} C_1 = 0, \quad z \geq 0, \quad r = a.$$

Step 2 can be carried out as described in [19], where a solution is given in terms of confluent hypergeometric functions of Kummer-type when $\bar{D} = 0$, as required by assumption A8. Finally step 3 requires considering the following boundary value problem:

$$v(r) \frac{\partial C}{\partial z} = \bar{D} \frac{\partial^2 C}{\partial z^2} + \frac{D}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) \tag{2.20}'$$

$$C(0, r) = C_0, \ \lim_{z \to \infty} C(z, r) \text{ exists} \tag{2.20}''$$

$$C(z, 0) \text{ is finite}, \quad D \frac{\partial C}{\partial r} = N(z), \tag{2.20}'''$$

where

$$N(z) := J(z) - \frac{kh_1}{k + h_1} C_1(z, 1) \tag{2.21}$$

and where subscript 2 has been omitted for the sake of notational simplicity.

Problem (2.20) was solved for constant N in [20] and approximate techniques of various sorts for dealing with general N were given in [21], [22]. See [23] for an analytical approach to (2.20) containing a rigorous analysis of the corresponding eigenvalue problem.

The foregoing formulation leading to (2.20) owes much to the general discussion in the opening paragraphs of [14]. Following that author's general recommendation, let's introduce dimensionless variables by means of the transformation

$$\tau = \frac{z}{a}, \quad \rho = \frac{r}{a}, \quad y = \frac{C}{C_0}. \tag{2.22}$$

Letting

$$2u(\tau) := \frac{aN(a\tau)}{DC_0}$$

and defining the dimensionless Peclet number by

$$P_e := \frac{a\bar{u}}{D}, \quad \bar{P}_e := \frac{D}{\bar{D}} P_e, \tag{2.23}$$

problem (2.20) transforms into

$$2(1-\rho^2)\frac{\partial y}{\partial \tau} = \frac{1}{P_e}\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial y}{\partial \rho}\right) + \frac{1}{\bar{P}_e}\frac{\partial^2 y}{\partial \tau^2} \qquad \tau > 0, 0 < \rho < 1 \tag{2.24}$$

$$y(0, \rho) = 1 \qquad 0 \le \rho \le 1 \tag{2.25}$$

$$\lim_{\tau \to \infty} y(\tau, \rho) \text{ exists} \qquad 0 \le \rho \le 1 \tag{2.26}$$

$$y(\tau, 0) \text{ is finite} \qquad \tau \ge 0 \tag{2.27}$$

$$\frac{\partial y}{\partial \rho} = 2u(\tau) \qquad \tau \ge 0, \quad \rho = 1. \tag{2.28}$$

An important special case obtains for very high axial Peclet number ($\bar{P}_e = \infty$, $\bar{D} = 0$), when (2.24) simplifies into

$$2(1-\rho^2)\frac{\partial y}{\partial \tau} = \frac{1}{P_e}\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial y}{\partial \rho}\right) \tag{2.29}$$

and (2.26) is no longer required. An initial boundary value problem is obtained by supplementing (2.29) by means of (2.25) and (2.27–28). This problem only will be considered in what follows. See [20] for an assessment of the goodness of this approximation, also [24] and [22] for approximate solutions to this problem.

3. MODEL SIMPLIFICATION

Just as model (2.17) above was characterized in terms of problem (2.18), problem (2.20) can be identified with a model differing from (2.17) in the choice of A, E, and hence Ω, but which one should be willing to identify with (2.17) anyway, considering how it originated. This should be understood implicitly in the sequel, whenever we refer occasionally to (2.17) in relation to this boundary value problem or even (2.24–28).

In the last few paragraphs of Sec. 2, we have "simplified" a model essentially by replacing Eq. (2.24) by Eq. (2.29). This type of operation is carried out with great frequency in applied mathematical practice, and we would like to devote some thoughts to it along with other model simplification procedures. Firstly, note that the character of the boundary value problem has been altered considerably. In fact, elliptic partial differential equation (2.24) has been replaced by (2.29), which is parabolic, thus rendering (2.26) unnecessary. Moreover, Eq. (2.24) does reduce to (2.29) for those solutions y (i.e., profiles) satisfying

$$\frac{\partial^2 y}{\partial \tau^2} = 0$$

so that this simplification amounts to replacing model (2.17) by

$$\langle T, S, A, \bar{E}, \bar{\Omega} \rangle \tag{3.1}$$

with

$$\bar{E} := \{e \in E : \partial^2 e / \partial z^2 = 0\}, \quad \bar{\Omega} := \bar{E}.$$

In general, model simplification will consist in replacing a model M as in (2.17) by a "simpler" model $\bar{M}$, with

$$\bar{M} := \langle \bar{T}, \bar{S}, \bar{A}, \bar{E}, \bar{\Omega} \rangle. \tag{3.2}$$

No attempt will be made here to formalize the meaning of "being simpler than" in this context. Instead, we shall content ourselves with regarding it as an extra-mathematical notion. See however [25].

Alternative simplification procedures obtain by taking limiting values of other parameters. For example, assuming $P_e = \infty$ in (2.24)—radial diffusion is offset by convective transport—leads to the ordinary differential equation parameterized by ρ:

$$\frac{\partial^2 y}{\partial \tau^2} - 2\bar{P}_e(1 - \rho^2)\frac{\partial y}{\partial \tau} = 0$$

with boundary conditions (2.25) and (2.26) plus the extra conditions (2.27) and (2.28). An elementary analysis shows that every solution of (2.24–26) satisfies also (2.27) as well as

$$\left.\frac{\partial y}{\partial \rho}\right|_{\rho = 1} = \infty,$$

hence (2.28) cannot be satisfied and the "simplified" problem has no solution.

Now the original problem (2.19–23) can be expected to have a unique solution [26, Vol. II, §IV.6] and yet its "simplified" version fails to even have a solution. Thus we see the need to be cautious when simplifying models.

An alternative simplification procedure was already illustrated by the change of variables (2.22) used to render the equations dimensionless. No loss of information is incurred in when doing so, because of the perfect reversibility of such relabeling (a nonsingular transformation from $\mathbf{R}^3$ into itself). Alternatively, consider the transformation

$$(\tau, \rho, y) \mapsto (t, z, x)$$

given on $\mathbf{R}^3$ by

$$t = \tau, \quad z = \rho^2, \quad x = y.$$

It leaves invariant the set $(0, \infty) \times [0, 1] \times \mathbf{R}$, and it is in fact invertible there, hence no loss of information can originate from using it. Yet the differential equation (2.29) simplifies into

$$(1 - z)\frac{\partial x}{\partial t} = \gamma \frac{\partial}{\partial z}\left(z \frac{\partial x}{\partial z}\right), \quad t > 0, \quad 0 < z < 1 \tag{3.3}$$

with initial condition

$$x(0, z) = 1, \quad 0 \leq z \leq 1 \tag{3.4}$$

and boundary conditions

$$x(t, 0) \quad \text{is finite,} \tag{3.5}$$

$$\frac{\partial x}{\partial z}(t, 1) = u(t), \quad t \geq 0, \tag{3.6}$$

where

$$\gamma := \frac{2}{P_e}. \tag{3.7}$$

Finally, it is worthwhile mentioning that all these models have been obtained once hypotheses A1–8 have been introduced. If any of these (stationarity, infinite length, linearity, and symmetry) conditions is removed, a more complicated model will arise which will, nevertheless, simplify into, say, (3.3–6) should we decide to. This hierarchical structuring of models is very much in the spirit of [14]. See also [27], where a hierarchy of models for heat conduction in a cylinder has been given. We shall concentrate very much in studying a model M specified by (3.3–6) in all that follows.

Zeigler in [3] has given a nice systematic account of valid model simplification using the language of mathematical system theory [2]. In [3], Zeigler considers a hierarchy of description levels and defines valid simplification at every level. One of these levels is that of *dynamical system* and we shall now concentrate exclusively on this level, referring the reader to chapters 9 and 10 of [3] for further enlightenment on these matters. Briefly, a system is an ordered collection

$$\langle T, U, X, Y, \mathcal{U}, \delta, \lambda \rangle, \tag{3.8}$$

where T, U, X, and Y are nonempty sets (of time instants, input values, internal states and output values, respectively) while δ and λ are functions (the state transition and the readout maps, respectively). Let us assume in what follows that T is an interval of real numbers, say $[0, \infty)$. Then $\mathcal{U}$ is a set of U-valued functions defined on T. For each $u \in \mathcal{U}$ and each subinterval $[a, b)$ of T, let u_{ab} denote the restriction of u to $[a, b)$ and let $\mathcal{U}_R$ denote the class of all such restrictions. Then $\delta : X \times \mathcal{U}_R \to X$ is subject to the following interpretation: $\delta(x, u_{sb}) :=$ state reached at instant t by applying input u over time interval $[s, t)$ assuming state at instant s was x.

Given this interpretation, a sensible restriction on δ is that it should have the following *composition property*:

$$\delta(x, u_{st}) = \delta(\delta(x, u_{sr}), u_{rt}) \tag{3.9}$$

for each choice of $s < r < t$.

Finally, $\lambda : X \to Y$ is subject to the interpretation

$$\lambda(x) := \text{output value when the state is } x.$$

Given a system Σ specified as in (3.8), a second system

$$\bar{\Sigma} := \langle T, U, \bar{X}, Y, \mathcal{U}, \bar{\delta}, \bar{\lambda} \rangle \tag{3.10}$$

is a *valid simplification* of Σ (in the sense of [3]) if there are onto mappings $\phi: X \to \bar{X}$, $\psi: Y \to Y$ such that the following relations hold:

(a) *Transition function preservation*

$$\bar{\delta}(\phi(x), u_{st}) = \phi(\delta(x, u_{st})) \tag{3.11}'$$

(b) *Output function preservation*

$$\bar{\lambda}(\phi(x)) = \psi(\lambda(x)) \tag{3.12}'$$

for each $x \in X$ and each $u \in \mathcal{U}$, $s < t$. Output function preservation clearly amounts to the commutativity relation

$$\bar{\lambda} \circ \phi = \psi \circ \lambda, \tag{3.12}''$$

where $\circ$ denotes function composition. Letting δ_{st} stand for map $x \to \delta(x, u_{st})$ for fixed $u \in \mathcal{U}$, $s < t$ (and similarly for $\bar{\delta}_{st}$) transition function preservation is clearly equivalent to the commutation relation,

$$\bar{\delta}_{st} \circ \phi = \phi \circ \delta_{st}. \tag{3.11}''$$

Note that both Σ in (3.8) and $\bar{\Sigma}$ in (3.10) have the same "purely external" elements, namely T, U, $\mathcal{U}$, and Y. In the terminology of [3], they are said to be *compatible*. Preservation relations analogous to (3.11) and (3.12) above can be defined for noncompatible pairs and this is done in [3]. We have decided to restrict ourselves to compatible pairs mainly for the sake of simplicity, but also because most cases of model simplification usually involve "simplifying" the state space and the state transition and readout maps only. See also [3] and [2] for more general definitions of system.

Model (3.1) specified by the initial boundary value problem (3.3–6) can be easily cast into a system like (3.8). For, taking into account the experimental observations reported in [17], it is clear that $N(z)$ in (2.21) is available from the experiment, while the radial profile $\{e(z, r), 0 \le r \le a\}$ at each location z is not. Moreover, classical theorems on parabolic partial differential equations [28] indicate that given any suitable smooth function u in (3.6) and any initial profile $\{x(0, z), 0 \le z \le 1\}$, there is a unique solution of (3.3) satisfying boundary conditions (3.5–6) and hence all future profiles $\{x(t, z), 0 \le z \le 1\}$ are well determined. Thus, it seems convenient to identify the following elements:

System terminology	*Experimental situation*
Time	Length along tube
Input value	Releasable agent rate of deposition
State	Radial concentration profile
Output value	Releasable agent rate of deposition.

Formally, let $T = [0, \infty)$, $U = Y = \mathbf{R}$ and define the state space as

$$X := \{x \in C^2(0, 1): x(0^+),\ x(1^-),\ x'(1^-) \text{ are defined}\}. \tag{3.13}$$

Let $\lambda: X \to Y$ be given by

$$\lambda(x) = x'(1) \tag{3.14}$$

and let $\mathcal{U}$ consist of all continuous functions $u: T \to U$. For each $v \in U$ let

$$X_v := \lambda^{-1}(v).$$

Finally, let operator A be defined on X by

$$Ax(z) = \frac{\gamma}{1 - z} \frac{\mathrm{d}}{\mathrm{d}z}\left(z \frac{\mathrm{d}x}{\mathrm{d}z}\right). \tag{3.15}$$

Then, from [28, §III.2] it follows that given $u \in \mathcal{U}$ and given $s < t$, $x \in X_{u(s)}$, there is a unique solution ξ of

$$\dot{x} = Ax \tag{3.16}$$

on $[s, t]$, satisfying

$$\xi(s) = x \tag{3.17}$$

$$\xi(r) \in X_{u(r)}, \quad s \leq r \leq t. \tag{3.18}$$

It only remains to set

$$\delta(x, u_{st}) := \xi(t), \tag{3.19}$$

and observe that δ satisfies (3.9) as a direct consequence of uniqueness, in order to complete the specification of model (3.3–6) as a dynamical system. Note that (3.16) is but a "more abstract" version of (3.3), that (3.4) corresponds with (3.17) in the particular case $s = 0$, $x(z) = 1$ for $0 \leq z \leq 1$ and that (3.6) has become (3.18)—see problem 2.1 in [1]. Analogous remarks apply to all the other models considered in Sec. 2.

A moment's consideration shows that all the successive scalings and changes of variable introduced in Sec. 2 (with the exception of those affecting the timelike variable) are of the type

$$\bar{x}(z) = ax(z^n/b^n), \quad 0 \leq z \leq b, \tag{3.20}$$

for $n = 1$ or $n = 2$, $a > 0$, $b > 0$, which results in ϕ linear and nonsingular given precisely by (3.20). Applied to the dynamical system just constructed, this requires modifying X in (3.13) into

$$\bar{X} := \{x \in C^2(0, b): x(0^+), x(b^-), x'(b^-) \text{ exist}\}. \tag{3.21}$$

Note that

$$\bar{x}(b) = ax(1), \bar{x}'(b) = \frac{na}{b} x'(1)$$

so that by (3.14) it suffices to take

$$\psi(y) = ay$$
$$\bar{\lambda}(\bar{x}) = \frac{b}{n}\bar{x}'(b)$$

to ensure the validity of (3.12). Note that ϕ is linear invertible (and denote it instead by P) so that (3.16) necessarily goes into a linear differential equation, say

$$\dot{\bar{x}} = B\bar{x} \tag{3.22}$$

with

$$B = PAP^{-1},$$

i.e.,

$$PA = BP. \tag{3.23}$$

The right state transition map $\bar{\delta}$ can be obtained as in (3.19)—working with (3.22) instead of (3.16)—and (3.11) can be seen to be equivalent to (3.23). This last relation can then be regarded as a preservation relation in its own right for this particular type of models.

Many other simplification procedures were mentioned in Sec. 2, some of them requiring elimination of terms in the differential equations or boundary conditions. There are many more procedures still which are of practical interest and frequent use [3, p. 39; 4]. Many (most?) of them are not valid in the sense of (3.11–12) but they can be shown to be valid in some approximative sense. Next section will be devoted to situations of this type, with special interest in space discretization.

4. DISCRETIZATION AND PRESERVATION RELATIONS

Let us focus on preservation relations of the type (3.23) with P linear but not necessarily invertible. Simplification procedures mapping X onto state spaces $\bar{X}$ "much simpler" than (3.21) will now be considered. Here the simplification will be achieved by choosing $\bar{X}$ to be a space of finite (or at most countable) dimension, instead of the infinite dimensional X in (3.21). This dimensionality reduction is to be held responsible for not having a preservation relation like (3.23) to hold exactly.

Let us begin by applying the familiar method of separation of variables to (3.3) in the very particular case when N in (2.21) is identically zero, i.e., $u(t)$ vanishes in (3.6). Then we are led to the eigenvalue problem [26, Vol. I, Chap. V]

$$(zu')' - \lambda(1-z)u = 0$$
$$u(0) \text{ defined}, \quad u'(1) = 0.$$

Following [19], let $v(\sqrt{-2\lambda}z) = \sqrt{z}u(\sqrt{z})$ to obtain an eigenvalue problem for v, with boundary condition

$$v(0) = 0 \quad v'(1) - v(1) = 0,$$

whose eigenfunctions are related to Whittaker's functions [29, Chap. XVI] $M_{k,0}(\alpha z)$, with k,

α functions of λ. The eigenvalues are the solutions of an equation of the form

$$aM_{k,0}(\alpha) + bM_{k+1,0}(\alpha) = 0$$

and they are all negative and countably many, say

$$-\omega_1^2, -\omega_2^2 \ldots$$

Let

$$\phi_1, \phi_2 \ldots \tag{4.1}$$

denote the corresponding normalized eigenfunctions. Hence any solution of (3.3), 3.5–6 with $u = 0$ is of the form

$$\xi(t, z) = \sum_{n=1}^{\infty} \bar{x}_n \, e^{-\gamma\omega_n^2 t}\phi_n(z). \tag{4.2}$$

Given any initial condition $x \in X$, the $\bar{x}_n$ are simply its Fourier coefficients with respect to the orthonomal systems (4.1) with inner product [26, Vol. I, Chap. V]

$$\langle f, g \rangle := \int_0^1 (1 - z) f(z) g(z) \, dz, \tag{4.3}$$

namely,

$$\bar{x}_n = \langle x, \phi_n \rangle. \tag{4.4}$$

Similar developments can be given for many other initial boundary value problems. They can be used in order to discretize the current model as indicated below.

Proceeding formally, let X be as in (3.13), then define

$$\bar{X} := \left\{ (\bar{x}_1, \bar{x}_2 \ldots) : \sum_{n=1}^{\infty} \bar{x}_n^2 < \infty \right\}$$

and let $P : X \to \bar{X}$ be given by

$$(Px)_n = \langle x, \phi_n \rangle, \quad n = 1, 2 \ldots \tag{4.5}$$

as in (4.3). Hence P is invertible, with

$$P^{-1}\bar{x}(z) = \sum_{n=1}^{\infty} \bar{x}_n \phi_n(z). \tag{4.6}$$

Applying P to A as in (3.15) in order to simplify (3.16) into (3.22), get

$$(PAP^{-1})\bar{x}_n = -\omega_n^2 \bar{x}_n, \quad n = 1, 2 \ldots$$

i.e.,

$$B = \operatorname{diag}(-\omega_1^2, -\omega_2^2 \ldots). \tag{4.7}$$

Hence (3.22) takes the particular form

$$\ddot{\bar{x}}_n(t) = -\omega_n^2 \bar{x}_n(t), \quad n = 1, 2 \ldots \tag{4.8}$$

which can be solved immediately, giving the simplified transition map $\bar{\delta}$ (for zero input only) in the form

$$\bar{\delta}(\bar{x}(0), 0_{0t}) = \bar{x}(t) \tag{4.9}'$$

with

$$\bar{x}_n(t) = x_n(0)\, e^{-\omega_h^2 t} \quad n = 1, 2 \ldots \tag{4.9}'''$$

Clearly (3.23) holds and there is complete preservation when discretizing by means of (4.5). However, this discretization requires zero input and leads into spaces which are still infinite dimensional. Let us simplify further in order to end up with finite dimensional systems of differential equations instead of (4.8).

To accomplish that one can proceed in a variety of ways. For example, system (4.8) can be truncated at $n = N$ obtaining

$$\xi_N(t, z) = \sum_{n=1}^{N} \bar{x}_n\, e^{-\gamma\omega_h^2 t} \phi_n(z)$$

instead of ξ in (4.2). However,

$$\xi_N(t, \cdot) \to \xi(t, \cdot) \text{ as } N \to \infty \tag{4.10}$$

in an appropriate sense provided each $\bar{x}_n$ is chosen as in (4.4). More formally, this amounts to choosing

$$\bar{X}_N := \mathbf{R}^N \tag{4.11}$$

and defining $P_N : X \to \bar{X}_N$ by

$$(P_N x)_i = \langle x, \phi_i \rangle, \quad i = 1 \ldots N. \tag{4.12}$$

Letting X_N stand for the linear subspace of X generated by $\phi_1 \ldots \phi_N$, it is clear that the whole orthogonal complement of X_N is mapped into the origin, hence P_N is singular. Therefore there is more than one choice of discretization A_N for A, and some of them may even fail to satisfy

$$P_N A = A_N P_N. \tag{4.13}$$

Truncation at $n = N$ requires taking

$$A_N = \operatorname{diag}(-\omega_1^2 \ldots -\omega_N^2) \tag{4.14}$$

and can be readily shown to satisfy (4.13). However, this choice of discretization is not very convenient from a practical viewpoint, as it requires a perfect knowledge of at least a finite segment of the spectrum of A. Hence in general, one would choose A_N to be another linear

operator of $\tilde{X}_N$, necessarily given by a real $N \times N$ matrix of elements $a_{ij}^{(N)}$, so that

$$(A_N \tilde{x})_i = \sum_{j=1}^{N} a_{ij}^{(N)} \tilde{x}_j. \tag{4.15}$$

However, choice (4.14) is readily characterized as the only one for which (4.13) holds. In general,

$$(P_N A x - A_N P_N x)_i + \omega_i^2 \langle x, \phi_i \rangle + \sum_{j=1}^{N} a_{ij}^{(N)} \langle x, \phi_j \rangle = 0$$

so that (4.13) will not be true for all P_N, although it may hold in the limit when $N \to \infty$ at least for some choices of $a_{ij}^{(N)}$ (see below).

Moreover, the same criticism made on (4.14) can be made on (4.12) as it requires knowing $\phi_1 \ldots \phi_N$, and this leads us to consider more general discretizations $P_N: X \to \tilde{X}_N$. Given that all operators involved in the original model are linear, it makes sense to restrict ourselves to linear continuous P_N. By Riesz' representation theorem [30, p. 110] for any such P_N there exist unique functions of bounded variation $\alpha_1 \ldots \alpha_N$ on [0, 1] such that

$$P_N x = \left(\int_0^1 x \, d\alpha_1 \ldots \int_0^1 x \, d\alpha_N \right). \tag{4.16}$$

Moreover, each discretization is in fact characterized by the choice of weighting functions $\alpha_1 \ldots \alpha_N$. Thus, (4.12) corresponds to

$$\alpha_i(z) = \int_0^z (1 - u)\phi_i(u) \, du. \tag{4.17}$$

A frequently chosen type of discretization is obtained by picking out the values of the function at selected points of its domain. This is done in this case by taking a partition

$$0 = z_0 < z_1 < \cdots < z_N = 1$$

of [0, 1] and letting, for $i = 1 \ldots N$

$$\alpha_i(z) = \begin{cases} 0 & 0 \le z < z_i \\ 1 & z_i \le z \le 1 \end{cases} \tag{4.18}$$

so that

$$(P_N x)_i = x(z_i) \quad i = 1 \ldots N. \tag{4.19}$$

The preservation relation in this case reduces then to

$$A x(z_i) = \sum_{j=1}^{N} a_{ij}^{(N)} x(z_i), \quad i = 1 \ldots N, \tag{4.20}$$

which is to hold for every $x \in X$. However, the usual finite difference methods involve

approximations of various sorts [31] based upon properties such as

$$x'(z) = \lim_{h \to 0} \frac{x(z+h) - x(z-h)}{2h} \tag{4.21}'$$

$$x''(z) = \lim_{h \to 0} \frac{x(z+h) - 2x(z) + x(z-h)}{h^2}. \tag{4.21}''$$

Assuming $z_i - z_{i-1} = h$ for all i, replacing the various derivatives in A by their approximants at each z_i according to (4.21) leads to

$$(A_N \bar{x})_i = \frac{\gamma}{2h} \frac{(2i-1)\bar{x}_{i-1} - 2i\bar{x}_i + (2i+1)\bar{x}_{i+1}}{1 - ih}, \quad 1 < i < N, \tag{4.22}$$

with appropriate choices for $i = 1$, $i = N$. However, instead of (4.20) one gets the limiting relation

$$Ax(z_i) = \lim_{N \to \infty} \sum_{j=1}^{N} a_{ij}^{(N)} x(z_i), \quad i = 1 \ldots N,$$

and in fact

$$\lim_{N \to \infty} \| P_N A x - A_N P_N x \|_N = 0, \text{ each } x \in X, \tag{4.23}$$

where $\| \ \|_N$ is any norm in $\mathbf{R}^N$. Let us now go back to the general case (4.16) and adopt the notation

$$(x, \alpha) := \int_0^1 x \, d\alpha$$

for $x \in X$, α of bounded variation. Hence (4.16) can be written as

$$(P_N x)_i = (x, \alpha_i), \quad i = 1 \ldots N, \tag{4.24}$$

just as (4.12). In fact, we will now present a discretization procedure that can be related to the method of separation of variables in which (4.12) originated. We will be looking for approximate solutions of (3.16) that can be written in the form

$$\xi_N(t, z) = \sum_{j=1}^{N} \bar{x}_j(t) \psi_j(z) \tag{4.25}$$

and for which (4.10) will be expected to hold. A collection of functions

$$\psi_1, \psi_2 \ldots \tag{4.26}$$

is given in X, not necessarily eigenfunctions associated with A. Then (4.25) may be thought of as the result of interpolating the values

$$\bar{x}_1(t) \ldots \bar{x}_N(t) \tag{4.27}$$

of $\xi_N(t, \cdot)$ at N specified locations of its domain. To be precise let us construct such

interpolation operation $Q_N: \bar{X}_N \to X$ by putting

$$Q_N \bar{x} = \sum_{j=1}^{N} \bar{x}_j \psi_j(z). \tag{4.28}$$

Note that

$$Q_N P_N x(z) = \sum_{j=1}^{N} (x, \alpha_j) \psi_j(z) \tag{4.29}$$

$$(P_N Q_N \bar{x})_i = \sum_{j=1}^{N} (\psi_j, \alpha_i) \bar{x}_j. \tag{4.30}$$

In particular, the choice in (4.18) leads to

$$Q_N P_N x(z) = \sum_{j=1}^{N} x(z_j) \psi_j(z) \tag{4.31}'$$

$$[P_N Q_N \bar{x}]_i = \sum_{j=1}^{N} \psi_j(z_i) \bar{x}_j. \tag{4.32}'$$

Note that

$$P_N Q_N = I_N \Leftrightarrow \psi_j(z_i) = \delta_{ij}; \quad i, j = 1 \ldots N \tag{4.32}''$$

$$Q_N P_N x = x \Leftrightarrow \psi_1 \ldots \psi_N \text{ solves the interpolation problem for } x \text{ on } z_1 \ldots z_N \text{ [32].} \tag{4.31}''$$

Very convenient choices of interpolation functions in (4.26) are the various kinds of spline functions [33], but they are by no means the only possibilities.

The discretization procedure will be arrived at through equation (3.16), by requiring (4.25) to be an approximate solution in the following sense: Compute the residual

$$R_N := \frac{\partial \xi_N}{\partial t} - A \xi_N,$$

namely,

$$R_N(t) = \sum_{j=1}^{N} \dot{\bar{x}}(t) \psi_j - \sum_{j=1}^{N} \bar{x}_j(t) A \psi_j. \tag{4.33}$$

Then specify weights

$$\beta_1 \ldots \beta_N \tag{4.34}$$

—integrators of bounded variation on [0, 1]—and require

$$(R_N(t), \beta_i) = 0 \quad i = 1 \ldots N. \tag{4.35}$$

This is the method of *weighted residuals* [34, 35]. It leads to

$$\sum_{j=1}^{N} (\psi_j, \beta_i) \dot{\bar{x}}_j(t) = \sum_{j=1}^{N} (A \psi_j, \beta_i) \bar{x}_j(t), \quad j = 1 \ldots N,$$

which is a linear system of ordinary differential equations. In the particular case in which

$$(\psi_j, \beta_i) = \delta_{ij}, \tag{4.36}'$$

we readily obtain

$$a_{ij}^{(N)} = (A\psi_j, \beta_i). \tag{4.36}''$$

If the weighting functions in (4.34) are chosen as those in (4.18), the resulting method is called *collocation* [24, 33, 34, 35, 36], and has been found to be very useful in the chemical engineering literature [37], [38, Vol. 2, §7.7]. Let us concentrate on this method, assuming (4.26)′ for the sake of simplicity, so that

$$a_{ij}^{(N)} = A\psi_j(z_i) \tag{4.37}$$

and both (4.31) and (4.32) hold, besides

$$\psi_j(z_i) = \delta_{ij}. \tag{4.38}$$

Note that

$$(P_N A x)_i = Ax(z_i),$$

$$(A_N P_N x)_i = \sum_{j=1}^{N} A\psi_j(z_i)x(z_j)$$

$$= A\left[\sum_{j=1}^{N} x(z_i)\psi_j\right](z_i)$$

because A is linear. Thus, (4.13) holds at x if

$$x = \sum_{j=1}^{N} x(z_i)\psi_j,$$

i.e., if $\psi_1 \ldots \psi_N$ solves the interpolation problem for x. Thus, (4.13) holds on the subspace X_N generated by $\psi_1 \ldots \psi_N$, but not necessarily on all X. In view of (4.31) and (4.32),

$$AQ_N = Q_N A_N \text{ on } \bar{X}_N \tag{4.39}$$

as well as the *approximate preservation relation*

$$P_N A = A_N P_N \text{ on } X_N. \tag{4.40}$$

Assuming (4.38), the discrete version of the operator A in (3.15) is then [24]

$$[A_N \bar{x}]_i = \sum_{j=1}^{N} \frac{\gamma}{1 - z_i} \frac{\mathrm{d}}{\mathrm{d}z}\left(z\frac{\mathrm{d}\psi_j}{\mathrm{d}z}\right)\Bigg|_{z=z_i} \bar{x}_j \tag{4.41}'$$

and the corresponding finite dimensional equation (3.22) is just

$$\dot{\bar{x}}(t) = A_N \bar{x}(t). \tag{4.41}''$$

To simplify matters, only homogeneous boundary conditions will be considered, i.e., $u(t) \equiv 0$ in (3.6). In this case the boundary conditions will be satisfied by each trial solution (4.25) provided

$$\psi_i'(1) = 0 \qquad i = 1 \ldots N.$$

Relation (4.40) can be shown to hold for the right choice of P_N, namely,

$$P_N x = (x(Z_n) \ldots x(Z_N))^T.$$

Observe that

$$X_1 \subset X_2 \subset \cdots \subset X_N \subset X_{N+1} \subset \cdots \subset X$$

and let

$$X_\infty := \bigcup_{n=1}^{\infty} X_n.$$

Then, given $x \in X_\infty$, there is a sufficiently large N such that

$$A_N P_N x = P_N A x,$$

so that

$$\lim_{N \to \infty} \| A_N P_N x - P_N A x \|_N = 0, \quad x \in X_\infty.$$

In general, however, X_∞ may be a proper subset of X, and the stronger conclusion

$$\lim_{N \to \infty} \| A_N P_N x - P_N A x \|_N = 0, \quad x \in X, \tag{4.42}$$

will not necessarily hold. Here, $\| \ \|_N$ denotes any norm in the finite dimensional space $\bar{X}_N$.

The convenience of one such strong limiting relation like (4.42) has already been pointed out in the Introduction, hence the importance of selecting the interpolation basis $\{\psi_n\}$ in such a way that $X_\infty = X$ in order to have convergence, i.e.,

$$\lim_{N \to \infty} \bar{x}^{(N)}(t) = x(t)$$

in an appropriate sense [see (1.10)]. See [39] and the bibliography listed therein for convergence analyses specially relevant to these applications.

In a more practical vein, one should mention that the dimension of (4.41) may be quite large, thus making it desirable to have A_N as simple (i.e., sparse) as possible, lest the computations become prohibitively cumbersome. Now the form of A_N depends on both the choice of interpolation basis and collocation points, $z_0, z_1 \ldots z_N$, hence choosing these points and functions in the "right" way is of considerable practical importance. In this connection, the use of spline and Hermite interpolation [33] and collocation at the zeroes of certain polynomials (as in orthogonal collocation [33, §8.7]) has been found most convenient for the sort of applications we have in mind [35, 36, 37]. Actual computations on the models constructed in Sec. 2 have been reported in [24], [21] and [37], among other sources.

5. CONCLUSIONS

An account has been given in Sec. 3 of valid simplification procedures for mathematical models, validity being expressed in terms of preservation relations, as in [3, Chap. 10]. However, the need to consider simplification procedures involving some sort of approximation cannot be overemphasized, in view of the considerable practical importance of such procedures. In [3, Chap. 13], Zeigler points out the need to undertake such a task, and Sec. 4 here is devoted to analyzing space discretization from this point of view, special emphasis being made on collocation and other weighted residuals type of techniques [35].

This is all done and illustrated with special reference to a mathematical model for transport phenomena and chemical reaction previously constructed in Sec. 2. The goodness of the approximation scheme is expressed in terms of the various elements in the original model, the simplified model and the discretization procedure satisfying an approximate preservation relation. Beside the theoretical importance of approximate preservation for modelling studies, it is known to have considerable practical importance as well, as it is shown in Sec. 4 to guarantee convergence of the predictions obtained from the simplified model to those afforded by the original model, provided the interpolation basis spans the whole space.

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REFERENCES

1. D. B. Hernandez, On some guiding principles in mathematical modelling with special emphasis on determinism. *Mathematical Modelling* **2**, 179–190 (1981).
2. L. Padulo and M. A. Arbib, *System Theory*, Saunders, Philadelphia, PA (1974).
3. B. P. Zeigler, *Theory of Modelling and Simulation*, Wiley, New York (1976).
4. J. C. Friedly, *Dynamic Behavior of Processes*, Prentice Hall, Englewood Cliffs, NJ (1972).
5. A. Belleni-Morante, *Applied Semigroups and Evolution Equations*, Clarendon Press, Oxford, England (1979).
6. H. F. Trotter, Approximation of semigroups of operators. *Pacific J. Math.* **8**, 887–919 (1958).
7. A. Pazy, Semigroups of linear operators and applications to partial differential equations. Math. Dept. Lecture Notes, Vol. 10, University of Maryland, College Park, MD (1974).
8. H. T. Banks and J. A. Burns, Hereditary control problems: Numerical methods based on averaging approximations. *SIAM J. Control Opt.* **16**, 169–208 (1978).
9. H. T. Banks and F. Kappel, Spline approximations for functional differential equations. *J. Diff. Eqs.* **34**, 496–522 (1979).
10. H. T. Banks and K. Kunisch, An approximation theory for nonlinear partial differential equations with applications to identification and control. LCDS Report 81-7, Brown University, RI (1981).
11. T. G. Kurtz, Extensions of Trotter's operators semigroup approximation theorems. *J. Functional Anal.* **3**, 354–375 (1969).
12. T. G. Kurtz, A general theorem on the convergence of operator semigroups. *Trans. Am. Math. Soc.* **148**, 23–32 (1970).
13. T. G. Kurtz, Approximation of population processes. Regional Conference Series in Applied Mathematics, Vol. 36, SIAM, Philadelphia, PA (1981).
14. R. Aris, Hierarchies of models in reactive systems, in *Dynamics and Modelling of Reacting Systems*, W. E. Stewart, W. H. Ray, and C. C. Conley, eds., pp. 1–35, Academic, New York (1980).
15. D. T. Huang and A. Varma, Yield optimization in a tube wall reactor. ACS Symposium Series No. 124, Computer Applications to Chemical Engineering (1980).
16. M. H. Fukami and L. Salgonicoff, Human platelet storage organelles: A Review. *Thromb. Haematostas.* **38**, 963–970 (1977).
17. G. A. Adams and I. Feuerstein, Platelet adhesion and release: Interfacial concentration of released materials. *Am. J. Physiol.* **240** (*Heart Circ. Physiol.* **9**), H99–H108 (1981).
18. R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, Wiley, New York (1960).
19. E. J. Davis, Exact solutions for a class of heat and mass transfer problems. *Can. J. Chem. Eng.* **51**, 562–572 (1973).
20. C. J. Hsu, An exact mathematical solution for entrance region laminar heat transfer with axial conduction. *Appl. Sci. Res.* **A17**, 359–376 (1967).

21. M. L. Michelsen and J. Villadsen, The Graetz problem with axial heat conduction. *Int. J. Heat Mass Transfer* **17**, 1391 (1974).
22. R. Siegel, E. M. Sparrow, and T. M. Hallman, Steady laminar heat transfer in a circular tube with prescribed wall heat flux. *Appl. Sci. Res.* **A7**, 386–392 (1957).
23. E. Papoutsakis, D. Ramkrishna, and H. C. Lim, The extended Graetz problem with prescribed wall flux. *AIChE J.* **26**, 779–787 (1980).
24. M. L. Michelsen, A fast solution technique for a class of linear partial differential equations. *Chem. Eng. J.* **18**, 59–65 (1975).
25. M. H. Schultz, The computational complexity of elliptic partial differential equations, in *Complexity of Computer Computations*, R. E. Miller and J. W. Thatcher, eds., pp. 73–83, Plenum, New York (1972).
26. R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Interscience, New York (1961).
27. D. B. Hernandez, Parameter lumping: When and to what extent?, Paper 9f of the 72nd Annual AIChE Conference, San Francisco, CA (1979).
28. S. D. Eidelman, *Parabolic Systems*, North Holland, Amsterdam (1969).
29. E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis*, Cambridge University, London, England (1965).
30. F. Riesz and B. S. Nagy, *Functional Analysis*, F. Ungar, New York (1955).
31. G. D. Smith, *Numerical Solution of PDE's: Finite Difference Methods*, Clarendon, Oxford, England (1978).
32. P. J. Davis, *Interpolation and Approximation*, Blaisdell, Waltham, MA (1963).
33. P. Prenter, *Splines and Variational Methods*, Wiley, New York (1975).
34. B. A. Finlayson and L. E. Scriven, The method of weighted residuals—A review. *Appl. Mech. Rev.* **19**, 735–748 (1966).
35. B. Finlayson, *The Method of Weighted Residuals and Variational Principles*, Academic, New York (1972).
36. J. V. Villadsen and W. E. Stewart, Solution of boundary value problems by orthogonal collocation. *Chem. Eng. Sci.* **22**, 1483–1501 (1967).
37. J. Villadsen, *Selected Approximation Methods for Chemical Engineering Problems*, Danmarks Tekniske Hojskole, Copenhagen, Denmark (1970).
38. R. Aris, *The Mathematical Theory of Diffusion and Reaction in Permeable Catalysts*, Clarendon, Oxford, England (1975).
39. J. Douglas, Jr. and T. Dupont, Collocation methods for parabolic equations in a single space variable, in Lecture Notes in Mathematics, No. 385, Springer-Verlag, New York (1974).